Stochastic Algorithms for Simulation and Analysis of Turbulent Premixed Combustion

John Bell

jbbell@lbl.gov
Center for Computational Sciences and Engineering
Lawrence Berkeley National Laboratory, USA
http://seesar.lbl.gov/ccse/

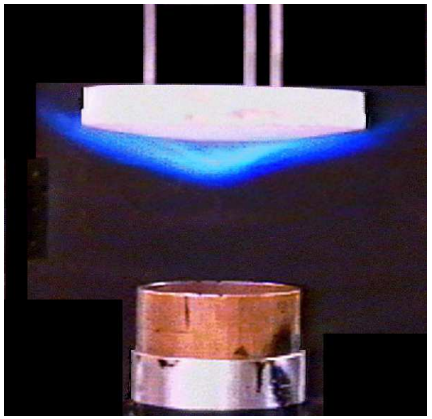
Presented at: Workshop on Front Propagation and Nonlinear Stochastic PDE's for Combustion and Other Applications
Universite de Montreal
January 26–29, 2005

Collaborators: V. Beckner, M. Day, J. Grcar, M. Lijewski
R. Cheng, M. Johnson, I. Shepherd

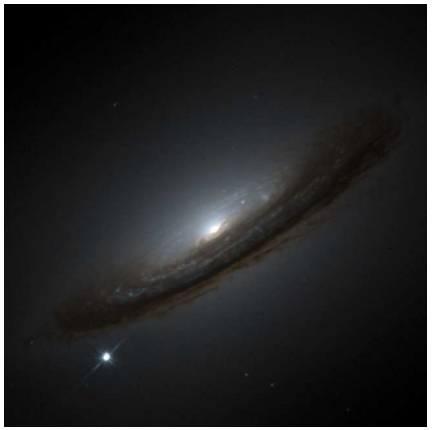
Turbulent Premixed Flames

Rod-stabilized V-flame

4-jet Low-swirl burner (LSB)



Stagnation flame



Type 1A supernova

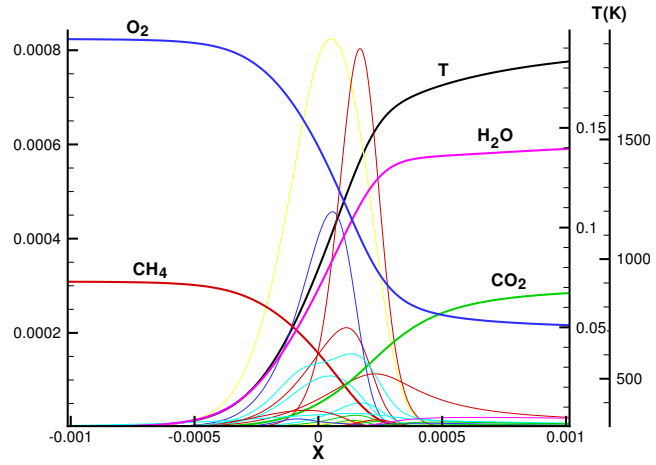
Premixed flames

Basic methane combustion

- $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O + \text{heat}$
- Multiple intermediate species, many reactions
- Initial reactions form radicals (chain initiating)
- Additional reactions multiply radical pool (chain branching)
- Radicals combine to form stable products (chain terminating)
- Requires heat to initiate reactions

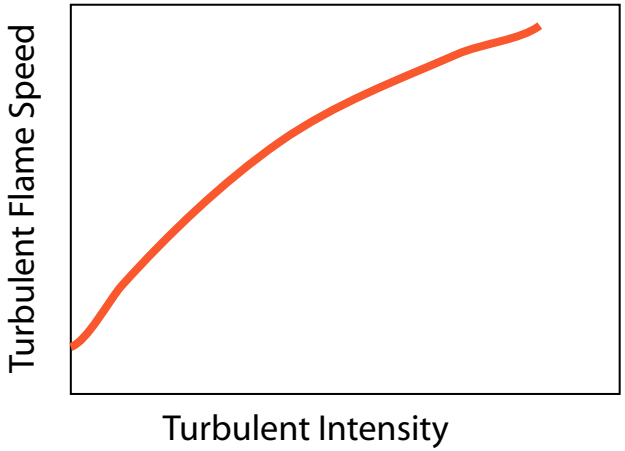
How does this work in a premixed flame?

- Released heat sustains reactions
- Heat and radicals formed "inside" the flame diffuse into fuel to initiate reactions
- Balance of diffusion and reaction

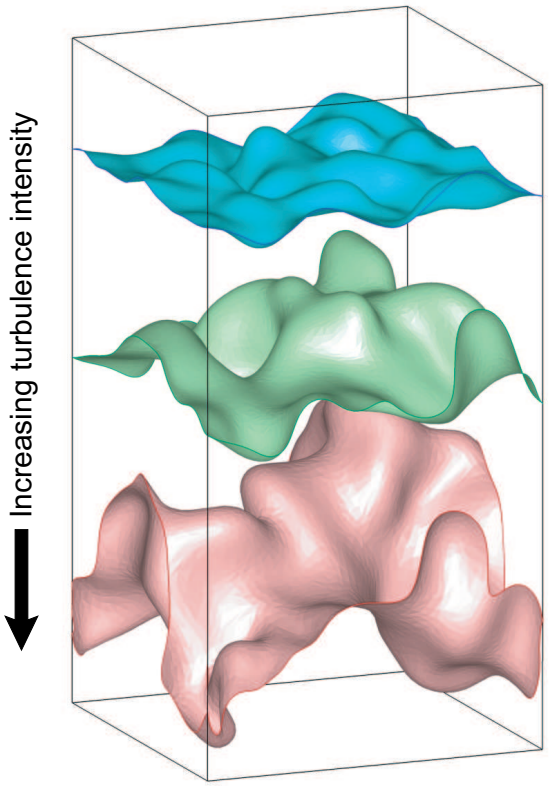


Effect of Turbulence

How does a premixed flame respond to turbulence?



- Turbulence accelerates flame
- Higher turbulent intensity leads to higher propagation speed



Flame propagating toward a source of turbulence is inherently unstable

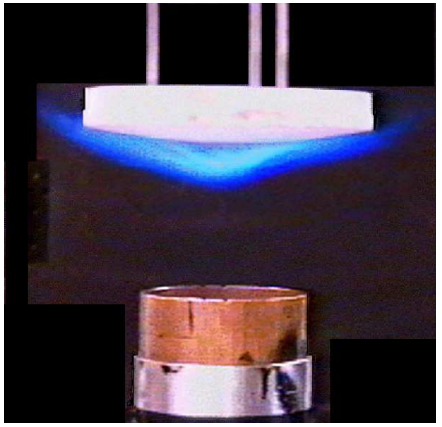
- $s_t < \bar{u} \rightarrow$ lower $u' \rightarrow$ lower s_t
- $s_t > \bar{u} \rightarrow$ higher $u' \rightarrow$ higher s_t

Turbulent Premixed Flames

Experimental flame stabilization mechanisms

Rod-stabilized V-flame

4-jet Low-swirl burner (LSB)



Stagnation flame

We would like to study these types of flames computationally

- Basic flame dynamics
- Turbulence / chemistry interaction

Inherent flame instability introduces complication

- How does stabilization effect the flame
- How should we stabilize the flame numerically

One possible approach

Simulate laboratory scale flame

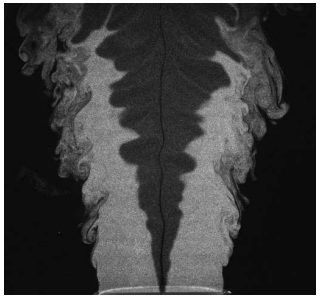
- Low Mach number formulation
- Detailed chemistry and transport
- Projection-based formulation
- Adaptive mesh refinement
- Dynamic load balancing

Issues:

- Simulation of stabilization
- Role of stabilization
- Characterization of boundary conditions
- Expensive

How do we effectively study premixed flames computationally

- How can we stabilize the flame computationally
- How can we understand the results



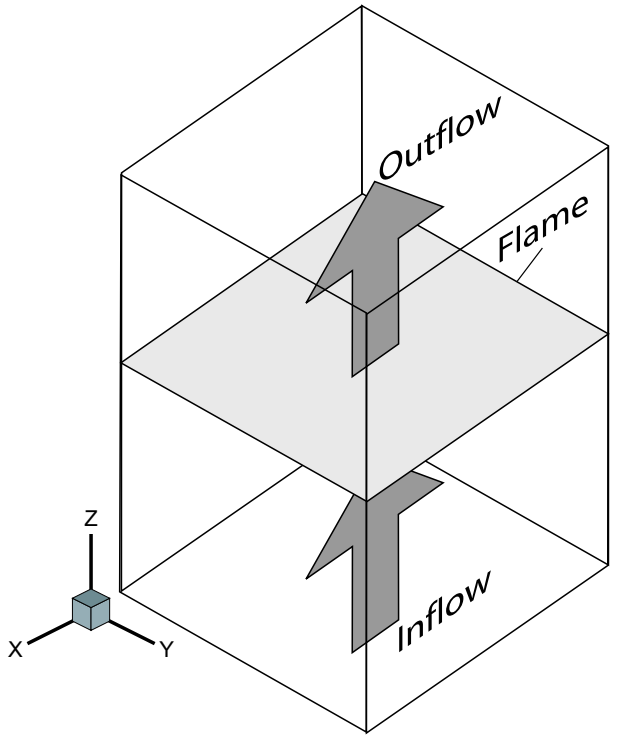
Simplified configuration

Most previous computational studies have used a simplified configuration

- Rutland and Trouve (1993)
- Trouve and Poinsot (1994)
- Zhang and Rutland (1995)
- Cant et al. (2002)
- Chakraborty and Cant (2004)
- Tanahasi et al. (2000,2002)
- Bell et al. (2002)

Unfortunately, this flame is unstable

Develop a computational approach to stabilize this flame and create a statistically stationary flame in this simplified geometry.



Turbulent flame sheet simulations

Automatic control

Dynamically adjust mean inflow velocity to stabilize flame

Assumptions

- Flame location defined as total mass of fuel in the domain
- There is an unknown turbulent flame speed $s(x)$ representing average speed of propagation that must be estimated
- Turbulent flame speed is not constant in time, it fluctuates around s

Stochastic ODE model

$$dx = (v_{in}(t) - s(x))dt + d\omega$$

Given an initial location of the flame $x(0) = \alpha$ and a target location β, find a strategy for adjusting $v_{in}(t)$ so that $x(t) \to \beta$ and estimate s

To model instability let $s(x) = \bar{s}(1 - \gamma(x - \beta))$

Want $v_{in}(t)$ to be smooth in time and positive

Control strategy

Introduce time scale τ that defines target time to reach control.

Want τ sufficiently large that $\int_t^{t+\tau} d\omega \approx 0$

Given $v_{in}(t_0)$ and s_{est} solve

$$\beta = x(t_0) + \int_{t_0}^{t_0+\tau} v_{in}(t_0) + (t - t_0)\Delta v - s_{est}\, dt = \tau(v_{in}(t_0) - s_{est}) + \tau^2 \Delta v/2$$

for slope Δv to define linear profile for $v_{in}(t)$ that controls the solution to the desired target

Adjust Δv so that maximum change in v_{in} is limited and $v_{in} > 0$

Use actual response of system to update s_{est}

$$s_{est} = (1 - \epsilon)s_{est} + \epsilon s_{obs}^{loc}$$

Control algorithm test

Test condition

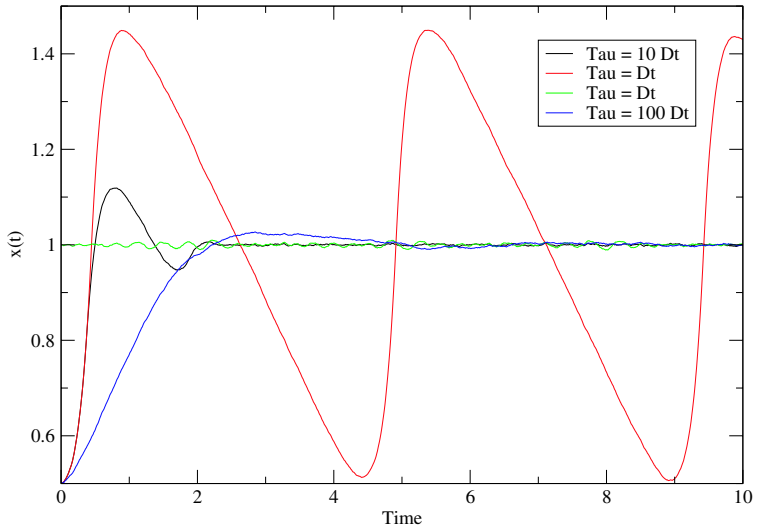
- $x(0) = .5, \quad \beta = 1.$
- $s = .3 - .1(x - 1.)$
- Noise $\approx 30\%$
- Max change 5%

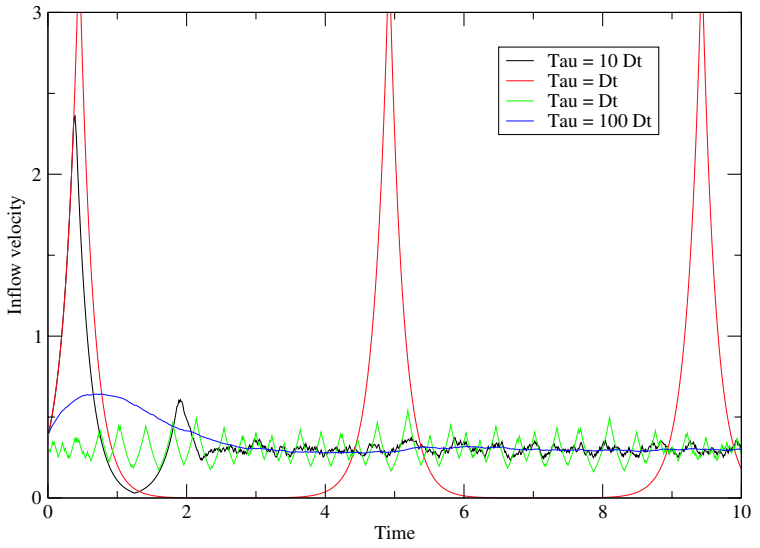
Comments

- Target interval to balance smoothness requirement
- Control insensitive to estimated speed
- Speed estimator noisy

For real flame calculations we observe

- Smooth temporal variation
- Noisiness in estimation



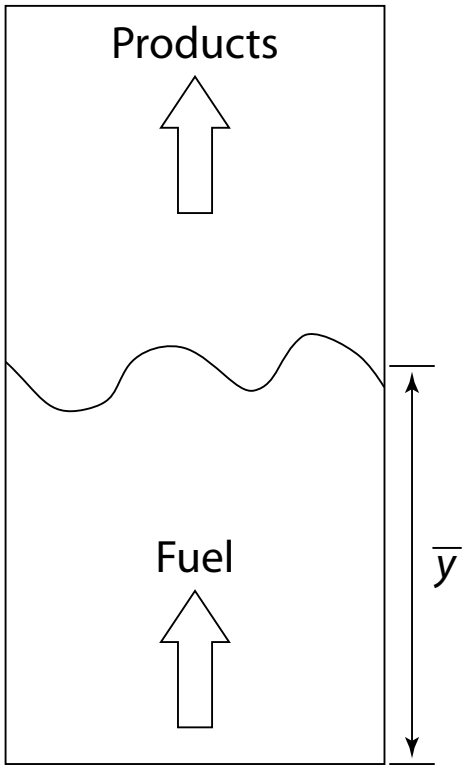


Flame Test Configuration

- 2D premixed CH_4 /air flame
- Low Mach code w/detailed chemistry and transport
- GRI Mech 3.0
  - 53 species
  - 325 reactions
- Inflow: $u = \bar{v}_{in} + w$

  $\bar{v}_{in}$ – mean inflow velocity

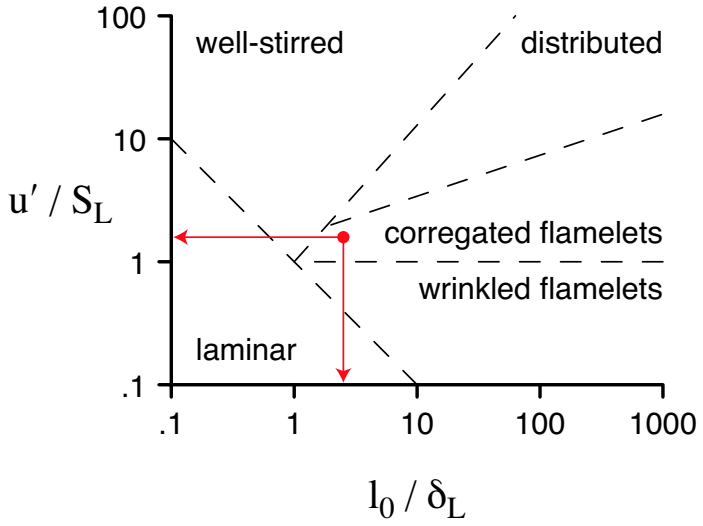
  w – "isotropic 2D turbulent fluctuations"



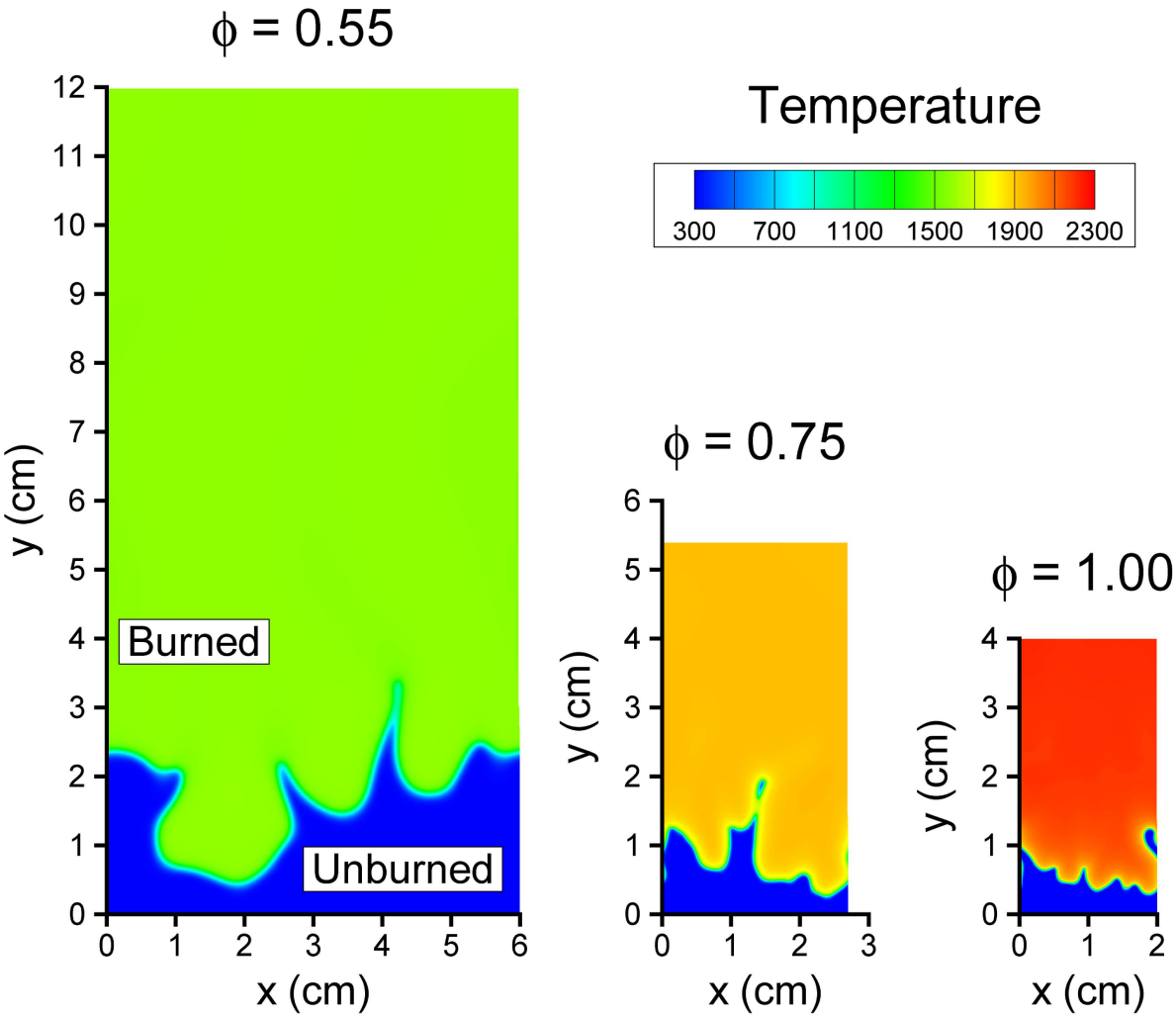
Demonstration Cases

Parameters:

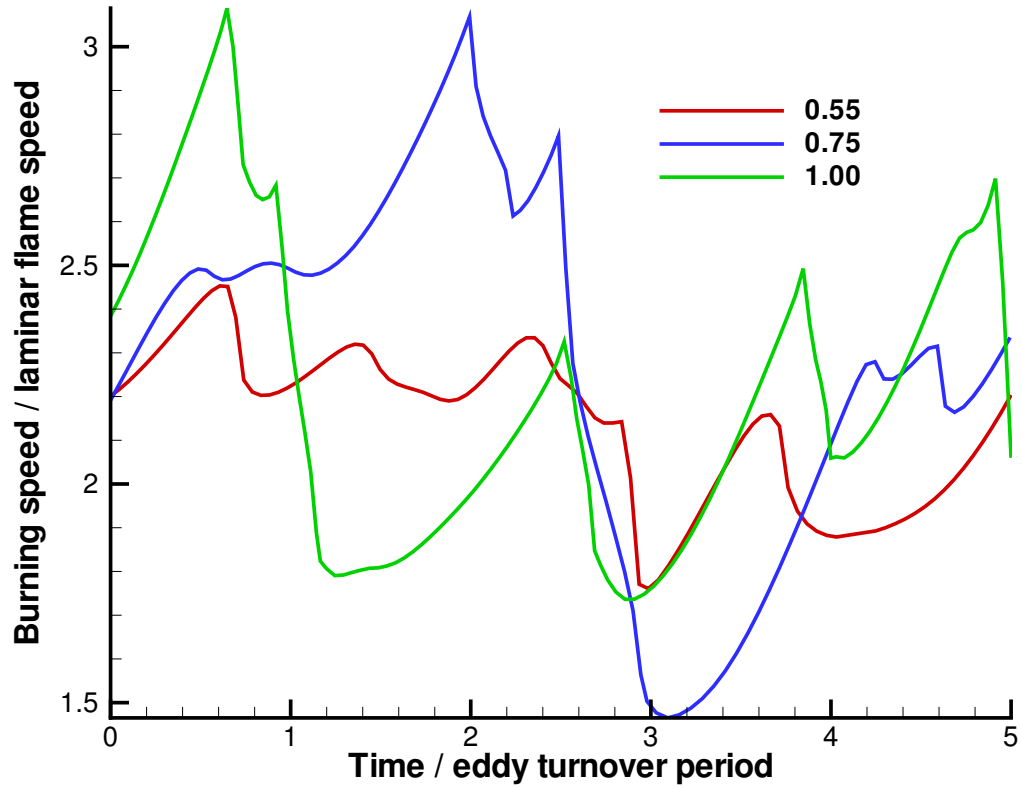
- ϕ = (0.55, 0.75, 1.00)
- $\ell_t \sim 2.6\delta_T$, $u' \sim 1.6 s_L$
- $L \sim 46\delta_T \sim 17\ell_t$
- $\Delta x = L/1024 \sim \delta_T/22$



Representative Snapshots



Turbulent flame speeds



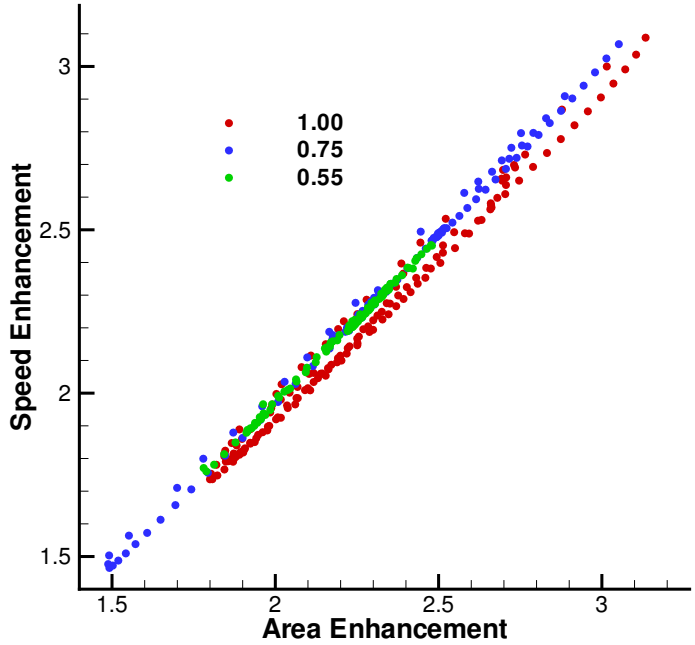
Global Analysis: s_L vs. A_T

s_T: **Fuel consumption rate**
Normalized by CH_4 mass fueling rate

s_L: **Laminar flame speed**

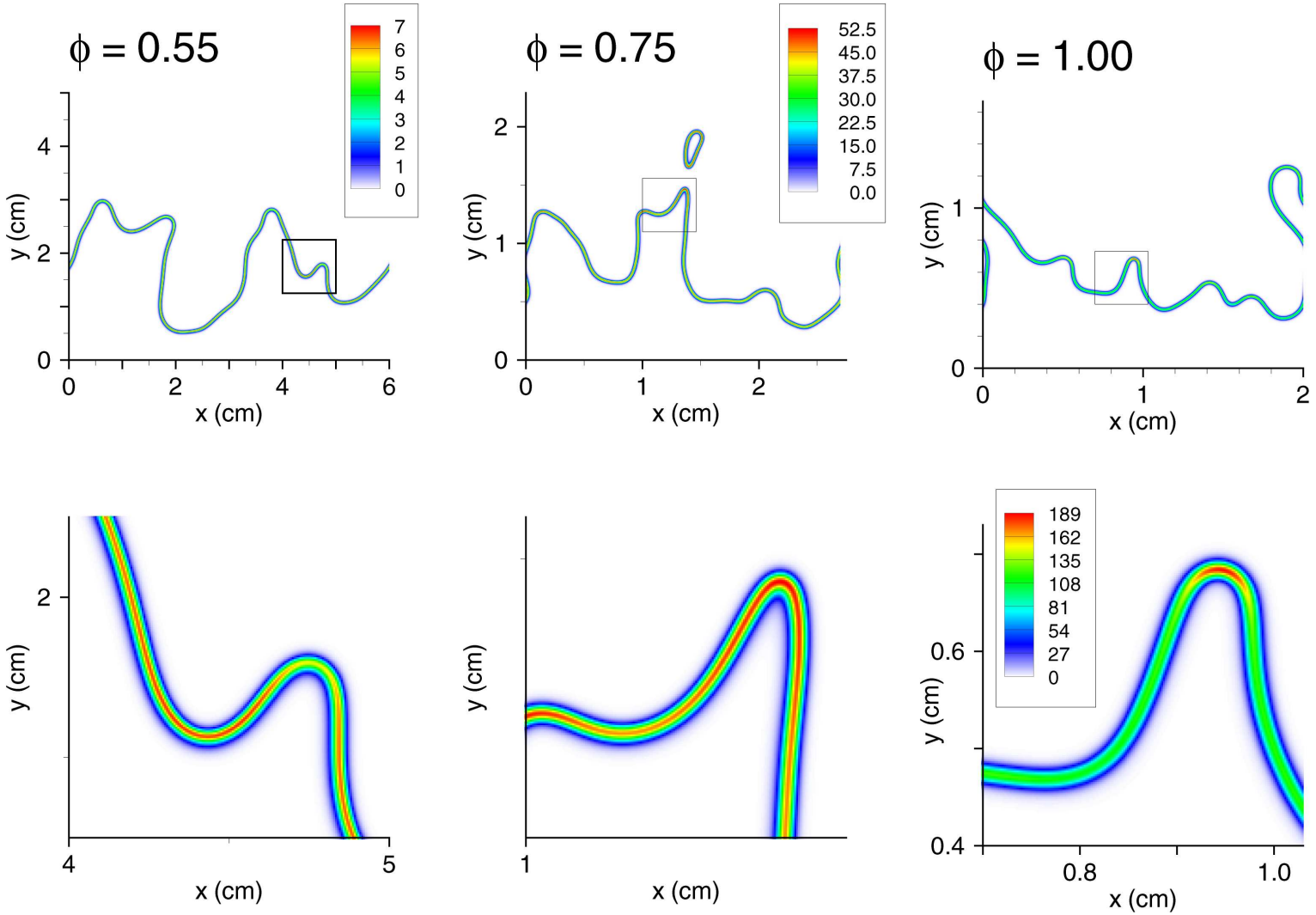
A_T: **Length of $T = T_{Q\,max}$ contour**
$T = T_{Q\,max}(\phi)$ is the temperature of peak heat release in flat flame.

L: **Width of domain**

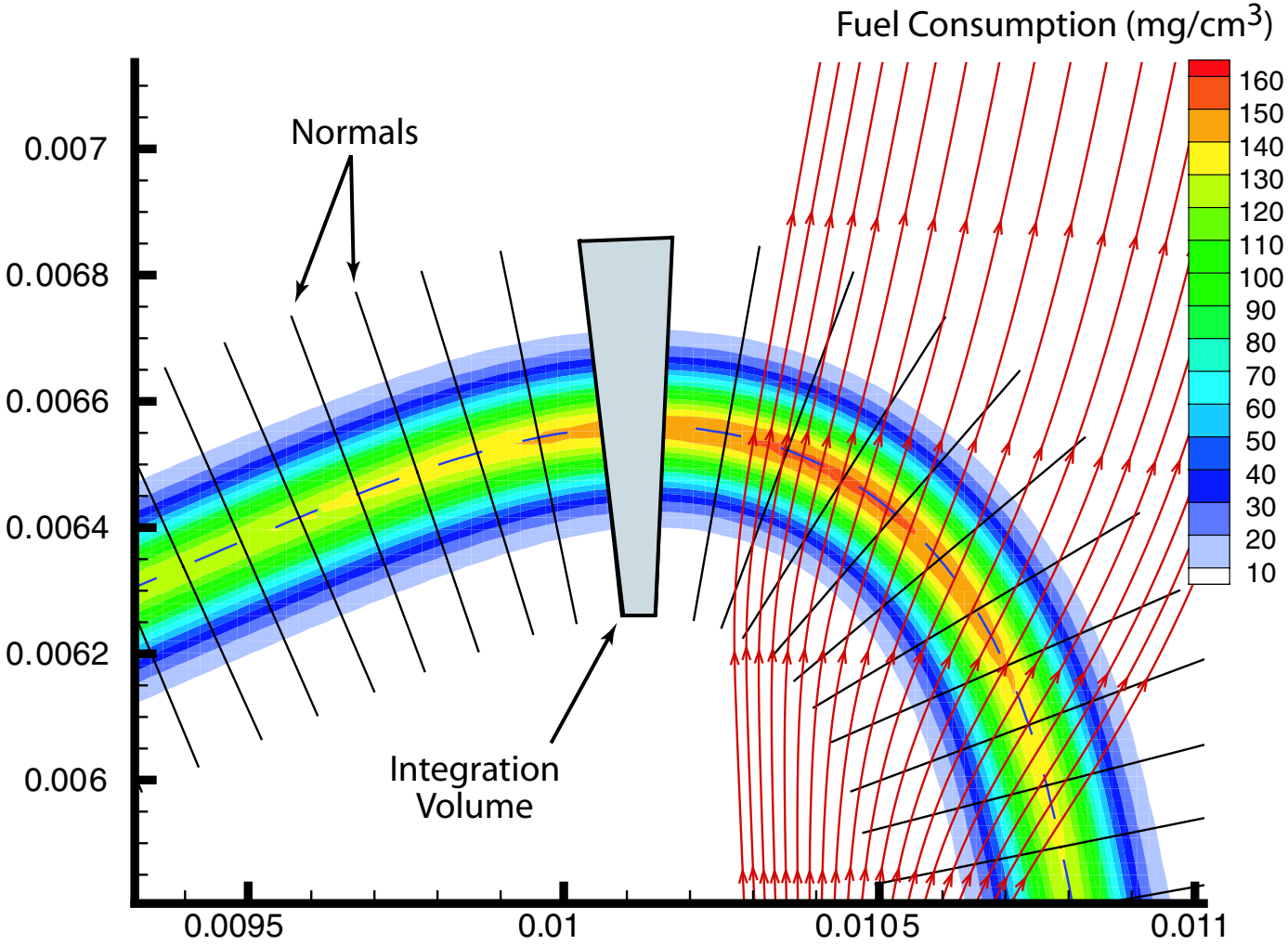


- Global consumption linear with flame area
- Flame area shows considerable variation

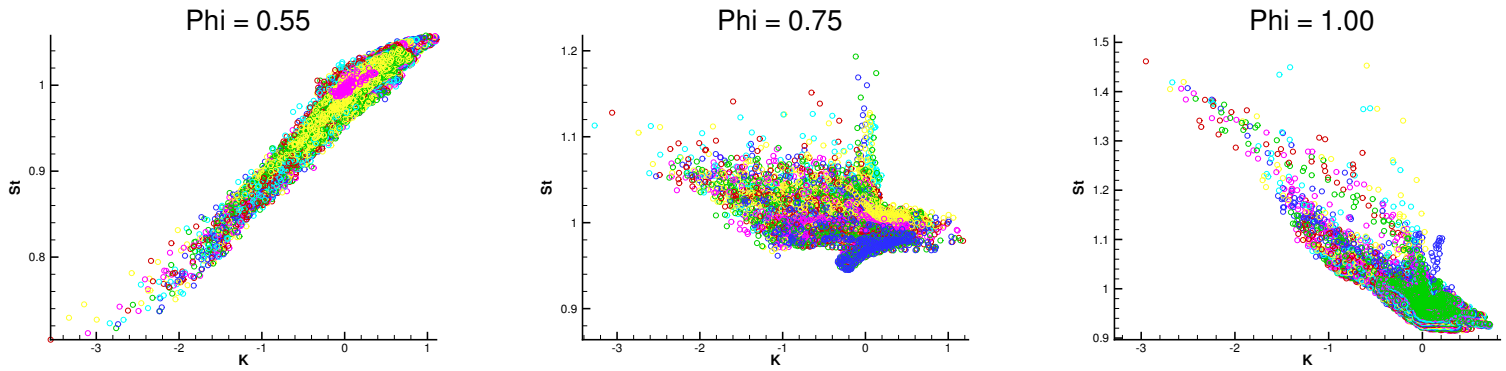
Consumption Rate Variability



Local estimates of s_T



Local consumption vs. curvature



- Opposite-sign correlation for ϕ = 0.55,1.00
- Is this linear? Looks as if slope changes at $\kappa = 0$
- Sections torn off do not have same Markstein variation

Flame diagnostics

How can we look in more detail at what is going on in these flames to explain observed behavior

Analysis of continuum data for multi-dimensional simulations is difficult, particularly for isolating chemical behavior

- Multiple processes
  - Advection
  - Diffusion
  - Reactions
- Cause and effect are difficult to separate

We want an easy way to pose and answer questions about the simulation

Experimental perspective: If you want to assess the chemical behavior of a system, tag specific atoms and monitor how they move through the system

For example, if we want to understand carbon chemistry in a methane flame, watch what happens to carbon atoms in the fuel.

- Carbon atom is transported by species (initially methane)
- Reactions transfer carbon from one species to another

Lagrangian formulation

We want to determine the fate of an atom A, initially in molecule, M_k

- Track trajectory of M_k
- If M_k reacts then A can move to another species $M_{k'}$

Eulerian form of species conservation:

$$\frac{\partial \rho Y_k}{\partial t} + \nabla u \rho Y_k = \nabla \rho D_k \nabla Y_k + \rho \omega_k$$

Lagrangian form of the species equation:

$$\rho \frac{DY_k}{Dt} = \frac{\partial Y_k}{\partial t} + u \cdot \nabla Y_k = \nabla \cdot \rho D_k \nabla Y_k + \omega_k$$

Stochastic formulation

Lagrangian form

$$\rho \frac{DY_k}{Dt} = \frac{\partial Y_k}{\partial t} + u \cdot \nabla Y_k = \nabla \cdot \rho D_k \nabla Y_k + \omega_k$$

Interpret species equations from the perspective of an atom A in molecule M_k

$$d\mathbf{x}_A = u(\mathbf{x}_A, t)dt + dW_{k(t)}(x_A, t) + dR_{k:k'}(x_A, t)$$

- W_k is a generalized Weiner measure (random walk) that represents effect of species diffusion
- $dR_{k:k'}(x_A, t)$ represents "scattering" of A in M_k into a set of other molecules $M_{k'}$ as a result of reaction

Ensemble of solutions gives behavior of tagged atoms

Model system using an operator split formulation

- Advection and diffusion
- Reactions

Advection / diffusion

Lattice approximation to random walk (1D)

$$\rho Y_k^{n+1} = \rho Y_k^n + \frac{\Delta t}{\Delta x^2}\left[(\rho D)^n_{k+1/2}(Y^n_{k+1} - Y^n_k) + (\rho D)^n_{k-1/2}(Y^n_{k-1} - Y^n_k)\right]$$

Given mass ρY_k at x_j, t^n,

$$\frac{\Delta t}{\Delta x^2}(\rho D)^n_{k-1/2} Y^n_k \text{ shifts left} \quad \text{and} \quad \frac{\Delta t}{\Delta x^2}(\rho D)^n_{k+1/2} Y^n_k \text{ shifts right}$$

Stochastic advection / diffusion:

$$\mathbf{x}^*_A = \mathbf{x}^n_A + \Delta t\, u$$

$$\mathbf{x}^{n+1}_A = \begin{cases} \mathbf{x}^*_A + \Delta x & \text{if } 0 \le \alpha \le p_R, \\ \mathbf{x}^*_A - \Delta x & \text{if } p_R < \alpha \le p_R + p_L, \\ \mathbf{x}^*_A & \text{if } p_R + p_L < \alpha \le 1. \end{cases}$$

For random number $\alpha \in [0, 1]$

Stochastic model of reactions

Elementary reactions

$$R1: \quad OH + CH_4 \Rightarrow CH_3 + H_2O$$

$$R2: \quad HCO + CH_4 \Rightarrow CH_3 + CH_2O$$

$$\frac{d[CH_4]}{dt} = -k_1[OH][CH_4] - k_2[HCO][CH_4]$$

Approximate differential equation using forward Euler

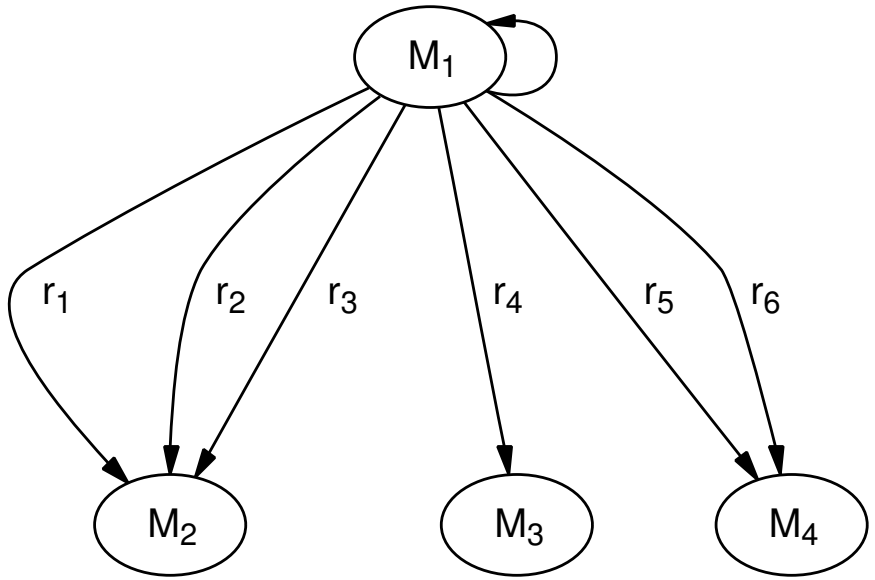
$$[CH_4]^{n+1} = [CH_4]^n - \Delta t\, k_1[OH]^n[CH_4]^n - \Delta t\, k_2[HCO]^n[CH_4]^n$$

Markov model

$$[CH_4]^{n+1} = [CH_4]^n - \Delta t\ k_1[OH]^n[CH_4]^n - \Delta t\ k_2[HCO]^n[CH_4]^n$$

Interpret as probabilities

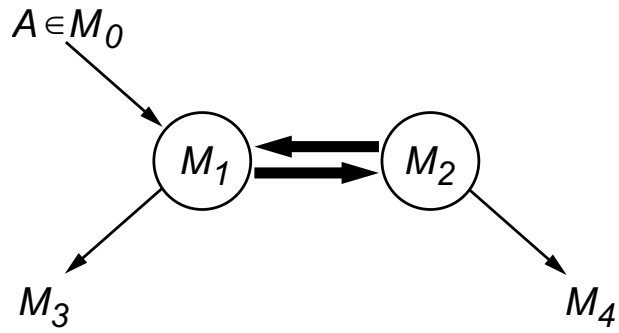
- $\Delta t\ k_1[OH]$ is probability of $CH_4 \rightarrow CH_3$ by R1
- $\Delta t\ k_2[HCO]$ is probability of $CH_4 \rightarrow CH_3$ by R2
- $1 - \Delta t\ k_1[OH] - \Delta t\ k_2[HCO]$ is probability CH_4 does not react



Model chemistry over Δt as a Markov process $\mathcal{M}^{\Delta t}$ subject to some subtleties

Formulation issues

Near equilibrium reactions



- Want $p(A) \approx p(B) \approx 0.5$
- Treat forward and reverse reactions separately

More formulation issues

Reaction ambiguity

Rxn 281: $CN + NO_2 \leftrightarrow NCO + NO$

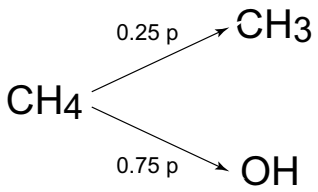
-O

-O, +C

Molecules with multiple atoms

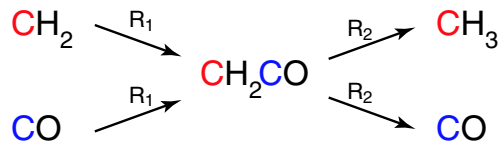
Rxn 11: $O + CH_4 \leftrightarrow OH + CH_3$

Probability = p



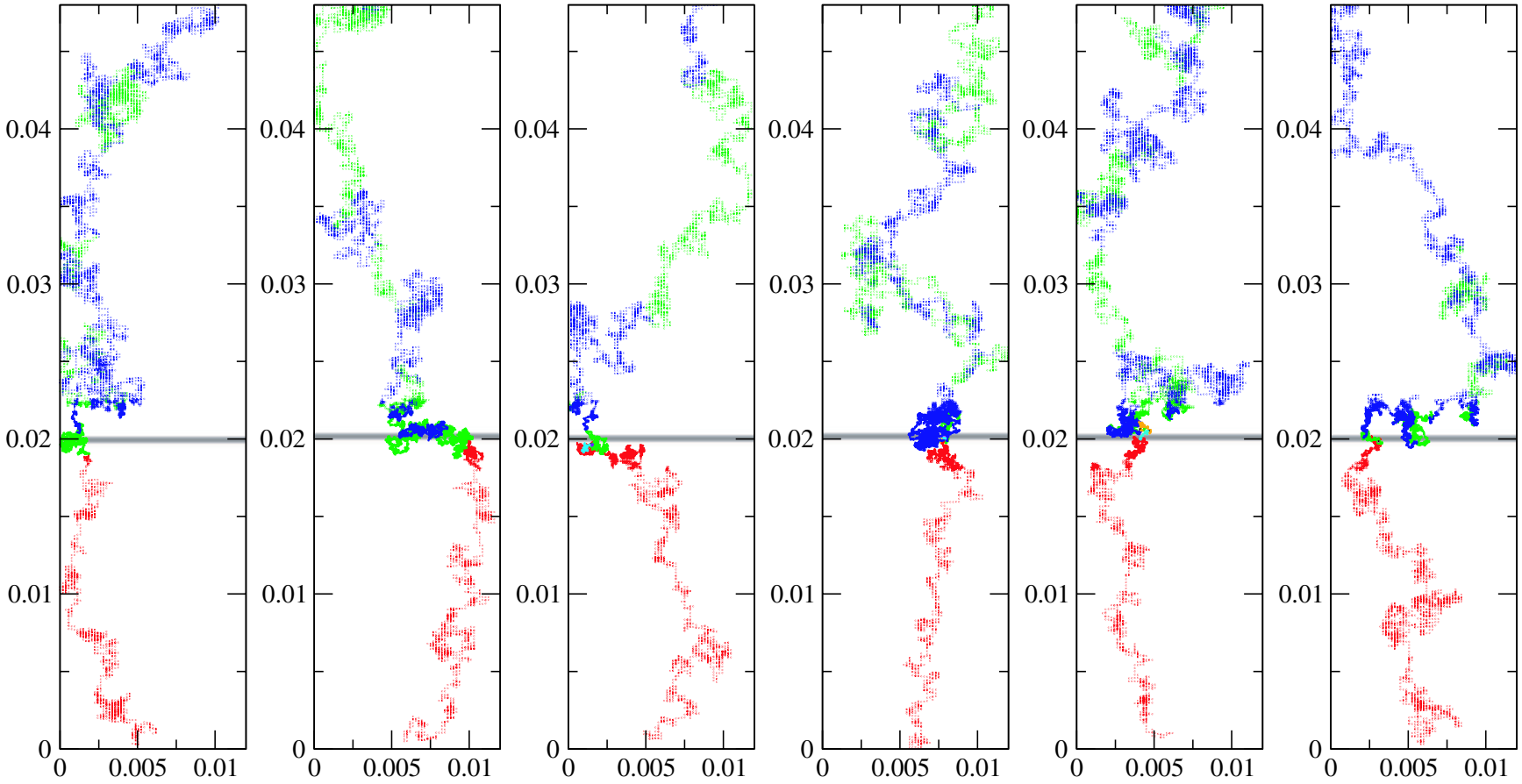
$CH_2 + CO(+M) \overset{R_1}{\leftrightarrow} CH_2CO(+M)$

$CH_2CO + H \overset{R_2}{\leftrightarrow} CH_3 + CO$



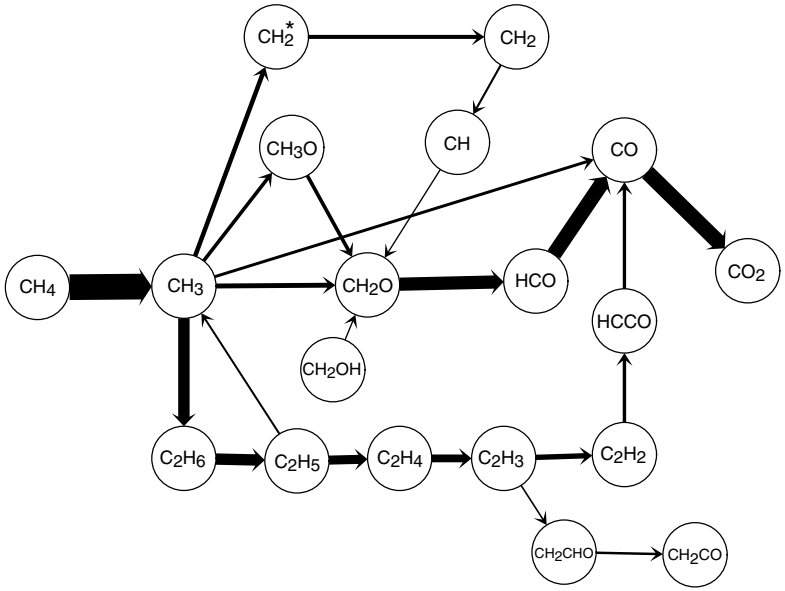
Steady premixed flame

Sample trajectories from steady premixed methane flame $\phi = 1.2$

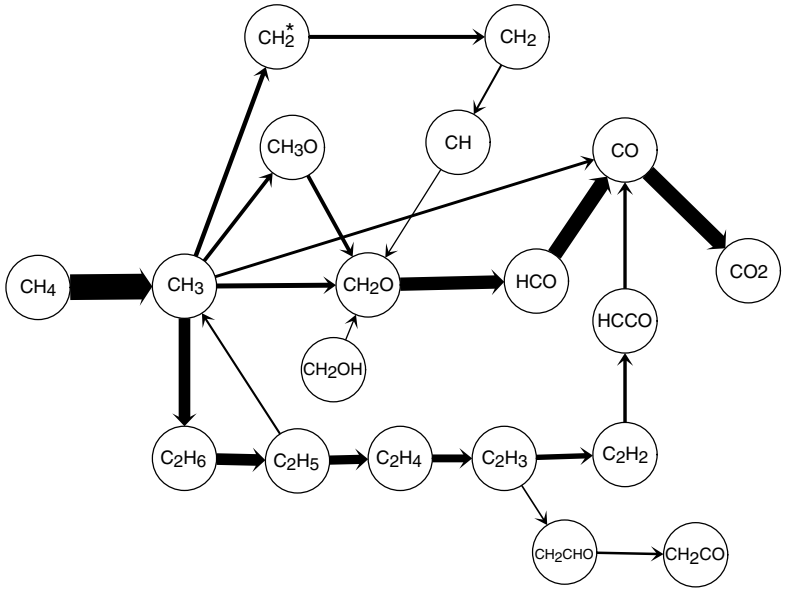


Premixed flame chemistry

Rich ($\phi = 1.2$) premixed methane flame computed using PREMIX with GRIMech 3.0



CHEMKIN rate evaluation



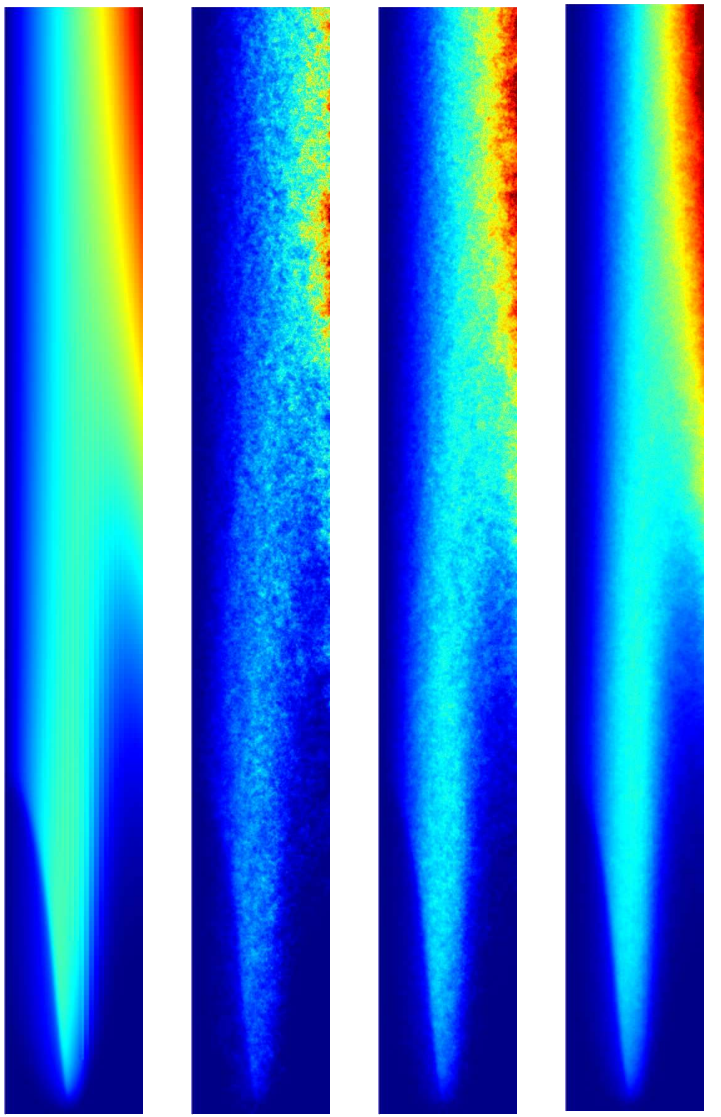
Tabulated chemisty from 80,000 particles

Spatial structure

Particle trajectories can also recover the spatial structure of the solution

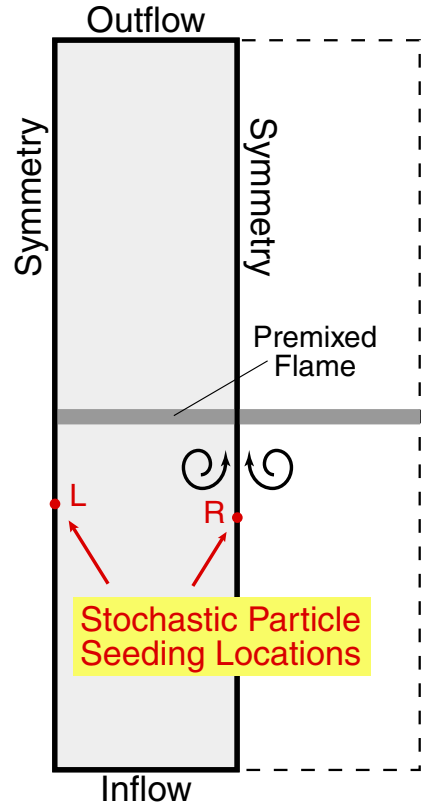
Laminar diffusion flame, specialized sampling to create trajectories

Ensemble average of the residence time of NO is proportional to the molar concentration (moles/area) of NO in the continuum solution



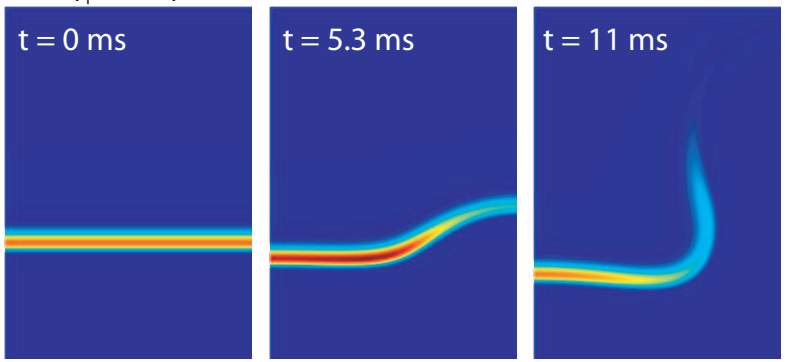
Vortex flame interaction

- Premixed CH_4-air fuel, N_2 -diluted
- $\phi = 0.8, 1.2$
- GRIMech 3.0
  - 53 species
  - 325 reactions
- Domain: 1.2 $\times$ 4.8 cm
- $\Delta x_{eff} = 47\mu$m

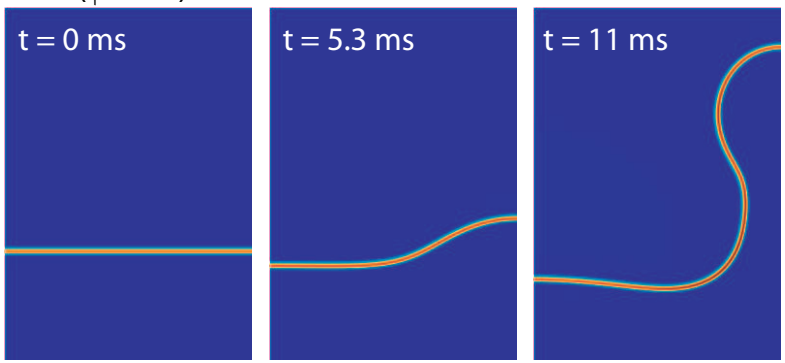


VFI chemistry

Rich ($\phi = 1.2$)

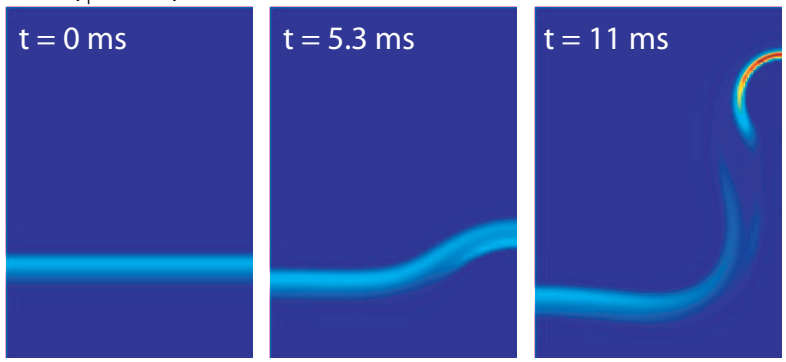


Lean ($\phi = 0.8$)

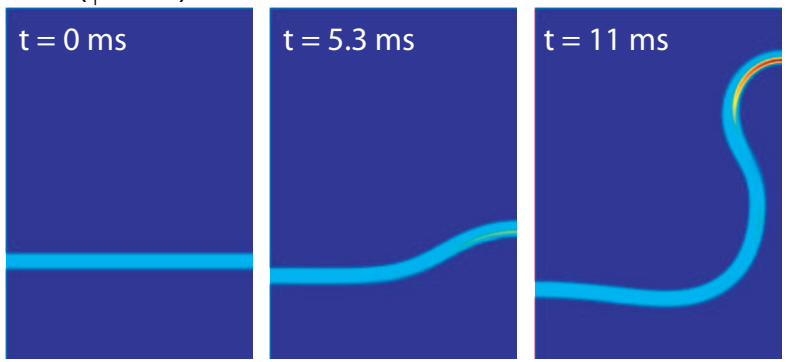


CH

Rich ($\phi = 1.2$)



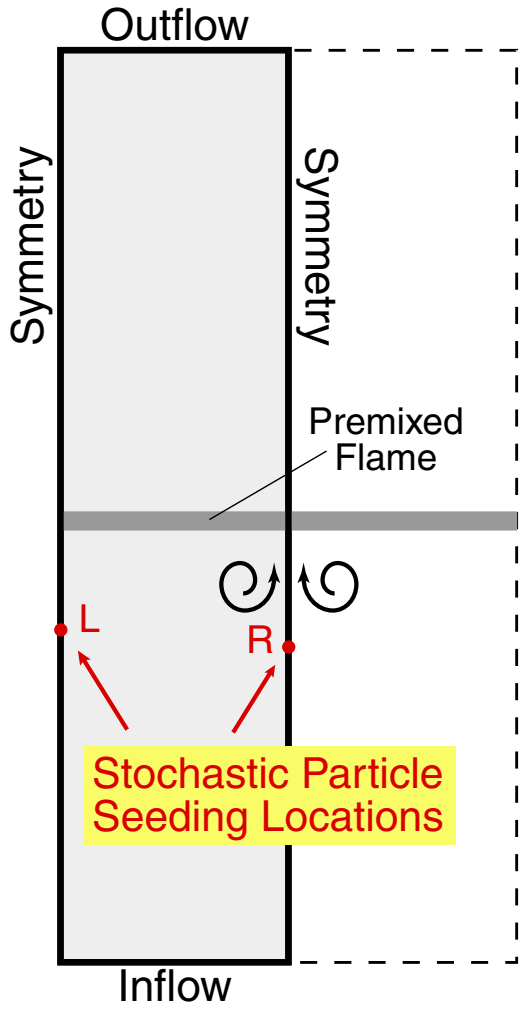
Lean ($\phi = 0.8$)



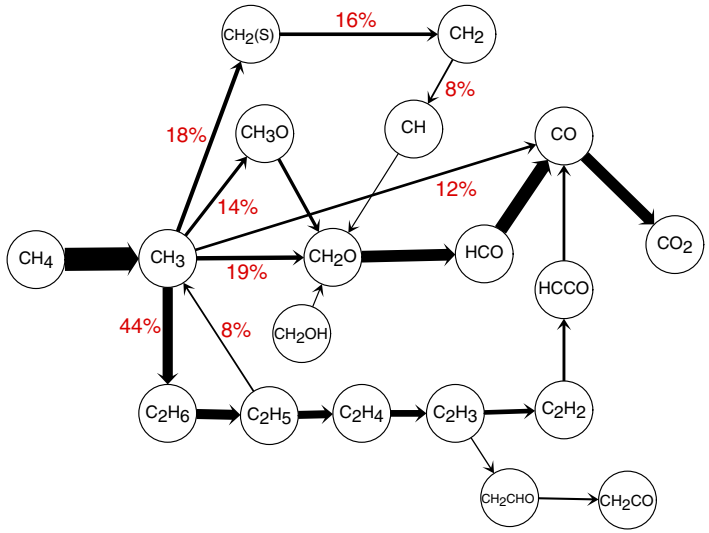
CH_3O

Stochastic particle analysis

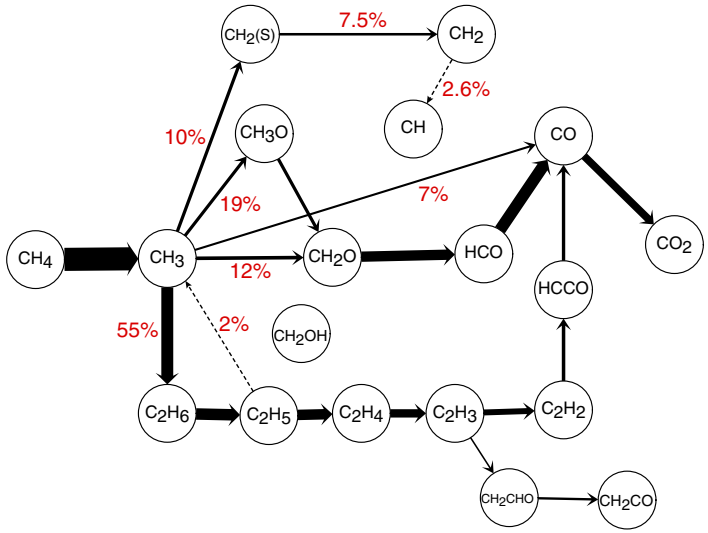
- Seed particles and L and R
- Collect an ensemble of trajectories
- Look at statistical behavior to analyze behavior



Reaction Path Diagrams - $\phi = 1.2$



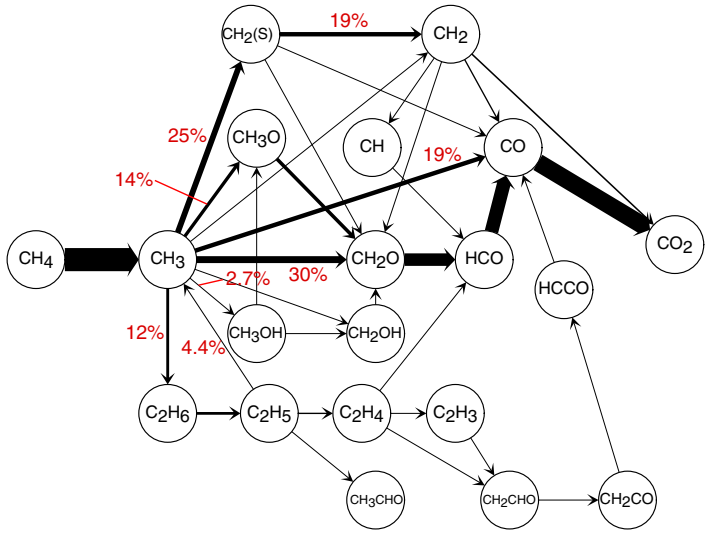
Left (strength $\geq$ 5%)



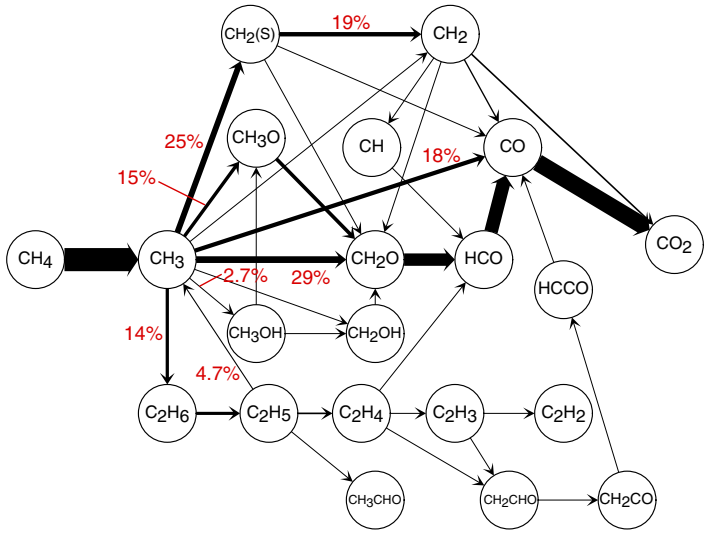
Right (strength $\geq$ 5%)

Dramatic shift away from $CH_3 \rightarrow CH_2^*$ pathway to $CH_3 \rightarrow C_2H_6$ pathway

Reaction Path Diagram - $\phi = 0.8$



Left (strength $\geq$ 1%)



Right (strength $\geq$ 1%)

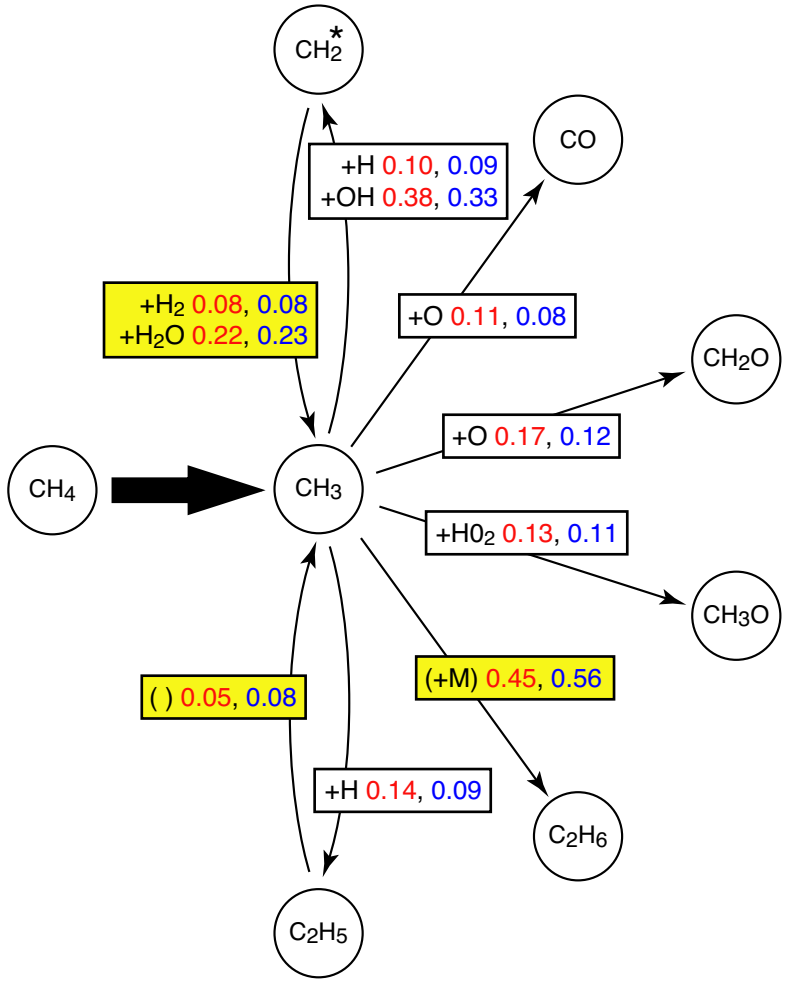
Pathways relatively unchanged in lean combustion

CH behavior

Why does interaction with vortex shift the chemical pathways

CH_3 chemistry

- Left – red
- Right – blue
- Yellow – no radicals



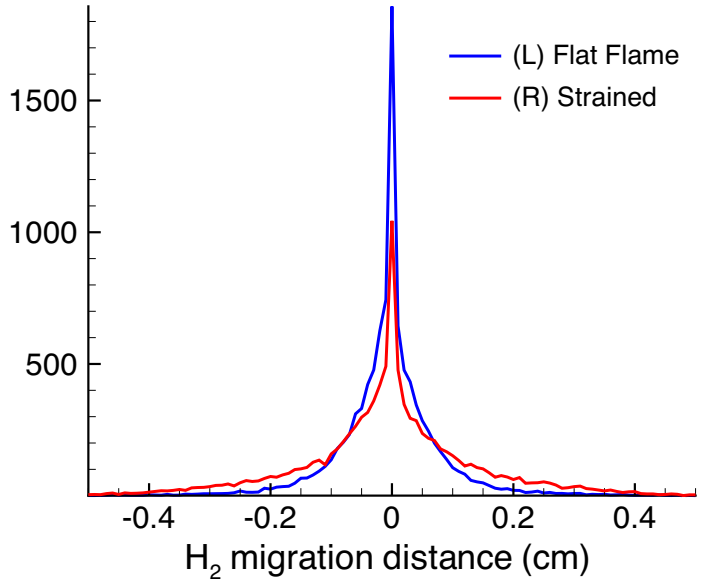
Shifting reaction pathways and reduced CH result from reduced radical pool

Radical behavior

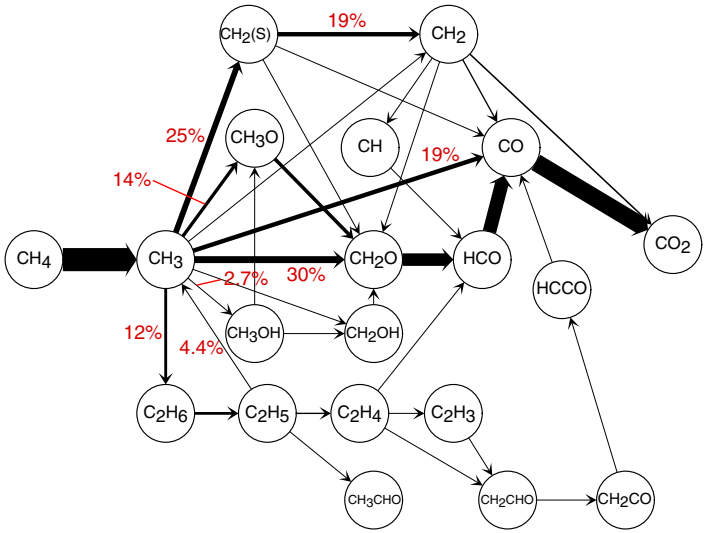
Classical flame theory suggests more mobile molecules, H and H_2, have the strongest effect on radical pool

Perform stochastic particle analysis for H-atoms

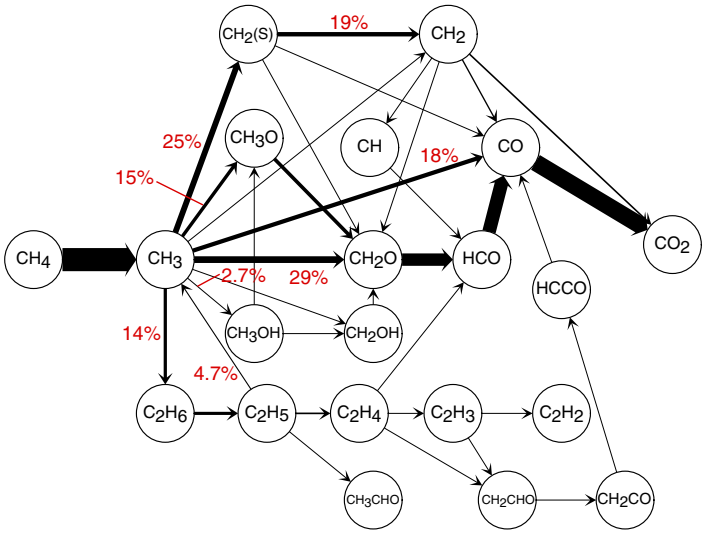
- H doesn't live long enough to be transported far
- H_2 life-expectancy more than doubles in strained region
- H_2 transported out of the flame zone



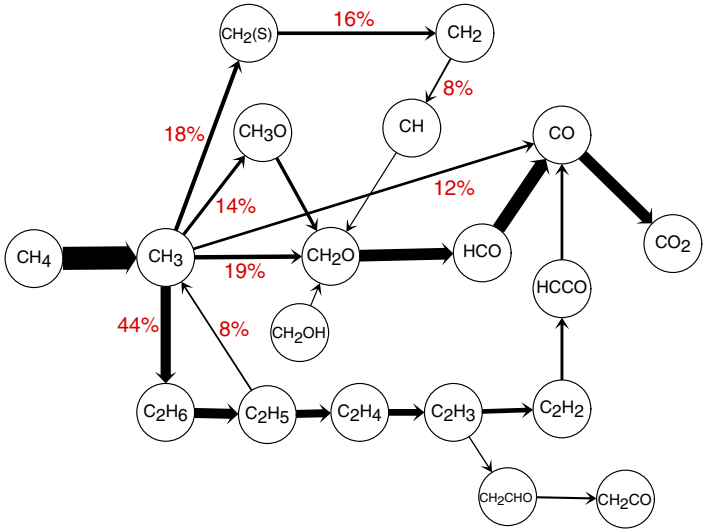
CH_3O



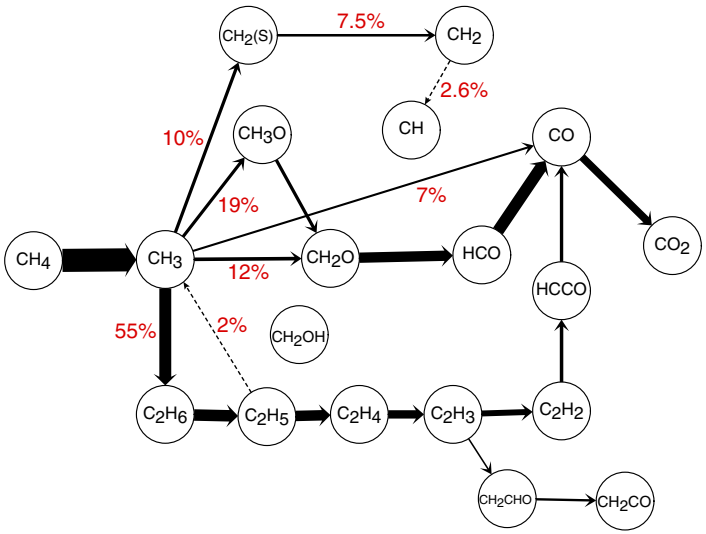
Left $\phi = 0.8$



Right $\phi = 0.8$



Left $\phi = 1.2$



Right $\phi = 1.2$

CH_3O behavior

CH_3O bloom is not a result of shifting pathways

Behavior of CH_3O is more subtle

Particle trajectories show two reactions destroy most of the CH_3O

$$Rxn\ 57: \quad CH_3O(+M) \rightarrow CH_2O + H(+M)$$

$$Rxn\ 170: \quad CH_3O + O_2 \rightarrow CH_2O + HO_2$$

- Molecules destroyed by Rxn 170 live on average more the a factor of two longer in the strained portion of the flame.
- Temperature profile is steeper where vortex interacts with flame
- CH_3O diffusing ahead of the flame sees colder conditions
- Rxn 170 is strongly temperature dependent ($T^{7.6}$)

CH_3O bloom is not a result of increased creation but increased longevity

Summary and future work

Stochastic algorithms in flame simulation

- Control of flames
  - Stochastic control algorithm
  - Smooth control for CFD coupling
  - Control based on time interval to reach target
- Stochastic particle diagnostics
  - Track "atoms" through the flow
  - Stochastic model for reactions and diffusion
  - Use ensemble of trajectories to investigate numerical solutions